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Geometrical Domain of Spin-1/2 Probability Mass Function

Abstract The quantum analogue of the classical characteristic function for a spin 1/2 assembly is considered and the probability mass function of the random vector associated with the assembly is derived. It is seen that the positive regions of Wigner and Margenau-Hill quasi distributions for the three components of spin, correspond to a trivariate probability mass function. We identify the domain of these positive regions as an Octahedron inscribed in the Bloch sphere with its vertices on the surface of the sphere. It is in this domain that a quantum characteristic function characterizing the quasi distribution, admits a probability mass function in IR^3 . It is also observed that the classical variates X_1 , X_2 , X_3 corresponding to the 3 spin operators σ_1 , σ_2 , σ_3 in the domain, are independent iff the Bloch vector lies on any one of the axes.

Keywords Spin-1/2 statistical assembly; Quasiprobability distribution

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1 INTRODUCTION

The study of quasiprobability distributions as quantum analogues to phase space distributions in quantum mechanical systems has been well documented [1]. These distributions have served as a very helpful tool in analyzing the statistical distributions of spinning submicroscopic particles like electrons, protons etc into various quantum mechanical states and also in providing insights into the connections between classical and quantum mechanics. The Wigner function gives the description of a quantum state in terms of a generalized function which acts a quantum analogue to probability distributions in particle phase space [2]. It was observed that this function assumed negative values in some domains of the phase space for certain quantum states. The Wigner function is hence a quasiprobability distribution for the position and momentum of a mechanical system determining the quantum state $\hat{\rho}$. The Sudarshan-Glauber's P distribution [3] [4] and the Husimi- Kano's Q distribution [5] [6], adopting a density matrix representation of the quantum state, have attempted to obtain distributions which correspond to positive, normalized classical distribution functions in phase space. But the Wigner,

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Sudarshan-Glauber P distribution and the Husimi- Kano Q distribution are not *genuine* classical probability distributions owing to the non-commutativity of the quantum mechanical operators which does not permit simultaneous measurement.

More recently, the quantum state reconstruction problem has been addressed using tomographic techniques on the Wigner function [7, 8, 9, 10, 11]. This technique uses quadrature histograms, which are radon transformations of the Wigner function. The Wigner function is consequently reconstructed from the histograms using the inverse Radon transformation known as marginal distributions [12]. Tomography has also been used in the measurement of spin states using positive normalized probability distributions wherein tomographic measurements of the density matrix for a quantum state are performed and the the method has been extended to measuring discrete spin operators [13]. The marginal distributions used in tomography play a central role in quantum state tomography and have even been considered as giving a classical-like representation of quantum systems [14]. Here, we explore the classical like nature of the phase space distributions of quantum mechanical systems by considering the Wigner and Margenau-Hill quasiprobability distributions.

Let us consider the spin vector $\overrightarrow{S}=(S_1,S_2,S_3)$ of the particle represented by $\frac{\hat{\sigma}}{2}=\frac{1}{2}(\sigma_1,\sigma_2,\sigma_3)$ in natural units where σ_1,σ_2 and σ_3 are the traditional Pauli's spin matrices satisfying the relations

$$\sigma_j^2 = I_2, \ \sigma_j \sigma_k = -\sigma_k \sigma_j, \ j \neq k = 1, 2, 3 \tag{1}$$

$$\sigma_1 \sigma_2 = i\sigma_3, \ \sigma_1 \sigma_3 = -i\sigma_2, \ \sigma_2 \sigma_3 = i\sigma_1$$

Each of these three matrices has eigen values ± 1 and consequently referred to as spin random vectors [15]. Given the state $|\Psi\rangle = a|1/2\rangle + b|-1/2\rangle$ of the particle, a classical measurement of the Cartesian components S_1, S_2 and S_3 of spin \overrightarrow{S} is given by the quantum mechanical expectation values

$$E_{QM}(\overrightarrow{S}) = \frac{1}{2} \langle \Psi, \hat{\sigma}\Psi \rangle$$
 (2)

The density matrix representation [16] [17] of the the quantum mechanical expectation values yields

$$E_{QM}(\overrightarrow{S}) = \frac{1}{2} Tr(\rho \hat{\sigma}) \tag{3}$$

where Tr implies the trace of the density matrix. The density matrix representation allows us to determine the measured value of the spin vector for a statistical assembly, which is given by the expectation value

$$E(\overrightarrow{S}) = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} Tr(\rho_i \hat{\sigma})$$
(4)

 $E(\overrightarrow{S})$ more specifically denotes the average of the quantum mechanical expectation values for the spin operators of the assembly. ρ_i refers to the individual density matrix associated with the i_{th} particle and N denotes the total number of particles in the assembly. Significantly, $E(\overrightarrow{S})$ may as well be writted in the form akin to equation (3) as

$$E(\overrightarrow{S}) = \frac{1}{2}Tr(\rho\hat{\sigma}) \tag{5}$$

where $\rho = \frac{1}{N} \sum_{i=1}^{N} \rho_i$ is referred to as the density matrix for the statistical assembly of spinning particles.

It is but natural to ask the question 'Can we identify these expectation values as moments of some statistical distribution?'. What we are looking for is a trivariate probability mass function $P(X_1 = x_1, X_2 = x_2, X_3 = x_3)$ of classical random variables X_1, X_2, X_3 corresponding to the three spin components, which must be able to reproduce exactly the expectation value $E(S_1, S_2, S_3)$ as given by equation (5). It is important, in this context, to keep in mind that S_1, S_2, S_3 are typically non commuting quantum mechanical observables. We identify the characteristic function of the random variables X_1, X_2, X_3 which corresponds to the spin operators at the expectation value level. In other words, the

three classical random variables correspond to the three spin operators in the sense that they produce the same expectation values. Further, it has been observed that in the pure state $|e_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$\phi(t_1, t_2) = \langle e_1, e^{(it_1\sigma_1 + it_2\sigma_2)} e_1 \rangle \tag{6}$$

is not a characteristic function of any probability distribution in the plane [18]. Parthasarathy also mentions the inconclusiveness of the conditions on a unit vector $|u\rangle$ and a family of observables X_1, X_2, \ldots, X_k in a Hilbert space \mathcal{H} , the function $\phi(t_1, t_2, \ldots, t_k) = \langle u, e^{(it_1X_1+it_2X_2+\ldots+it_kX_k)}u\rangle$ is in IR^k . In this paper, we look to identify the conditions and consider the quantum analogue of the classical characteristic function $(E(e^{(it_1X_1+it_2X_2+it_3X_3)})$ [19] for a spin half assembly and identify the domain in which it admits a trivariate probability mass function in IR^3 . In section 3 we take into consideration the interesting Bloch vector $\overrightarrow{p}=(p_1,p_2,p_3)$ and parameterize the density matrix using the Bloch vector and state the conditions for pure and mixed states ensembles. In section 4, we briefly discuss the Wigner-Weyl and Margenau-Hill quasiprobability distribution functions and the rules which associate a classical characteristic function to the corresponding quantum mechanical operator and identify the geometrical domain in which the Margenau-Hill characteristic function admits a probability mass function for the quantum spin 1/2 assembly.

2 SPIN -1/2 DENSITY MATRIX

For a mixture state the density matrix ρ is given by

$$\rho = \sum_{k=1}^{N} w_k |\Psi_k\rangle \langle \Psi_k| \tag{7}$$

where $w_k = N_k/N$ is the probability of finding the particle in the state $a_k|1/2\rangle + b_k|-1/2\rangle$ and N_k stands for the number of particles in the state $|\Psi_k\rangle$. Since the density matrix ρ is Hermitian and $Tr(\rho)$ is normalized to unity, only three real parameters and hence three measurements are necessary to specify ρ in its entirety. It is customary to represent the density matrix of a spin-1/2 system by

$$\rho = \frac{1}{2} (I_2 + \sigma_1 p_1 + \sigma_2 p_2 + \sigma_3 p_3)$$

$$= \frac{1}{2} \begin{pmatrix} 1 + p_3 & p_1 - ip_2 \\ p_1 + ip_2 & 1 - p_3 \end{pmatrix}$$
(8)

The Bloch vector \overrightarrow{p} is given by

$$p_k = Tr(\rho \sigma_k) = 2E_{QM}(S_k) \tag{9}$$

Since the density matrix is positive semidefinite with the diagonal entries representing probabilities, we have for mixed states

$$p_1^2 + p_2^2 + p_3^2 \le 1 \tag{10}$$

Since the density operator for pure states is idempotent, it can be easily verified that

$$Tr(\rho^2) = (Tr\rho)^2 = 1 \tag{11}$$

in other words,

$$p_1^2 + p_2^2 + p_3^2 = 1 (12)$$

Clearly, for mixture states $Tr(\rho^2) < 1$ and consequently the state of polarization of a spin 1/2 assembly may be represented by a point within the sphere

$$p_1^2 + p_2^2 + p_3^2 < 1 (13)$$

3 DOMAIN OF DISTRIBUTION FOR SPIN-1/2 ASSEMBLY

The correspondence between an observable in quantum probability and a random variable in classical probability has been recognized [18]. These observables in general, are non-commuting and represented by Hermitian matrices. Of the various correspondence rules which associate classical quantities to quantum mechanical operators [20], the Wigner-Weyl correspondence rule [1] characterizing the Wigner quasiprobability distribution can be stated as

$$e^{(At_1+Bt_2)} \to e^{(\mathbf{A}t_1+\mathbf{B}t_2)} \tag{14}$$

or

$$A^m B^n \to \{ \mathbf{A}^m \mathbf{B}^n \} \tag{15}$$

where A and B represent the classical variates and A and B represent non-commuting quantum mechanical operators. The $\{\}$ stands for the total symmetrizer with (m+n)!/m!n! terms. It can be noted that $\phi(t_1,t_2)=\langle e_1,e^{i(\sigma_1t_1+\sigma_2t_12)}e_1\rangle$ considered in [18], follows the Wigner-Weyl association rule for a bivariate distribution. In a trivariate case for a more general ρ , $\phi(t_1,t_2,t_3)$ can be written as

$$\phi(t_1, t_2, t_3) = Tr(\rho e^{i(\sigma_1 t_1 + \sigma_2 t_2 + \sigma_3 t_3)}) = \cos(\|\overrightarrow{t}\|) + i \frac{\langle \overrightarrow{p}, \overrightarrow{t} \rangle}{\|\overrightarrow{t}\|} \sin(\|\overrightarrow{t}\|)$$

$$\tag{16}$$

where $\|\overrightarrow{t}\|$ denotes the norm of the vector $\overrightarrow{t} = (t_1, t_2, t_3)$.

The Margenau-Hill [1] symmetrization rule can be written in the form

$$e^{i(At_1+Bt_2)} \to \frac{1}{2} \left(e^{i\mathbf{At}_1} e^{i\mathbf{Bt}_2} + e^{i\mathbf{Bt}_2} e^{i\mathbf{At}_1} \right) \tag{17}$$

or equivalently

$$A^m B^n \to \frac{1}{2} (\mathbf{A}^m \mathbf{B}^n + \mathbf{B}^n \mathbf{A}^m)$$
 (18)

It is to be noted that the moments obtained from the Margenau-Hill and the Wigner-Weyl distributions are the same for a spin 1/2 assembly. We hence consider the Margenau-Hill distribution and identify the domain in which the quantum characteristic function for the distribution admits a trivariate probability mass function in IR^3 .

Generalizing equation (17) for three spin operators, the characteristic function is defined as [19]

$$\phi(t_1, t_2, t_3) = \frac{1}{3!} (\rho(\lambda_{123} + \lambda_{132} + \lambda_{213} + \lambda_{231} + \lambda_{312} + \lambda_{321}))$$
(19)

where

$$\lambda_{abc} = e^{i\sigma_a t_a} e^{i\sigma_b t_b} e^{i\sigma_c t_c} \tag{20}$$

Using equations (1),(8),(9) together with the relations

$$e^{i\sigma_k t_k} = I_2 \cos(t_k) + i\sigma_k \sin(t_k); k = 1, 2, 3$$
$$\langle \hat{\sigma}, \overrightarrow{A} \rangle \langle \hat{\sigma}, \overrightarrow{B} \rangle = \langle \overrightarrow{A}, \overrightarrow{B} \rangle + i\langle \hat{\sigma}, (\overrightarrow{A} \times \overrightarrow{B}) \rangle$$
(21)

where (\times) refers to the vector cross product, we can simplify equation (19), which yields

$$\phi(t_1, t_2, t_3) = \cos(t_1)\cos(t_2)\cos(t_3) + ip_1\sin(t_1)\cos(t_2)\cos(t_3) + ip_2\cos(t_1)\sin(t_2)\cos(t_3) + ip_3\cos(t_1)\cos(t_2)\sin(t_3)$$
(22)

Upon inverting the above equation and obtaining the three independent moments for the trivariate distribution, we find that it is the characteristic equation of a discrete trivariate random vector (X_1, X_2, X_3) with a probability mass function

$$P(X_1 = x_1, X_2 = x_2, X_3 = x_3) = \frac{1}{8}(1 + x_1p_1 + x_2p_2 + x_3p_3)$$
(23)

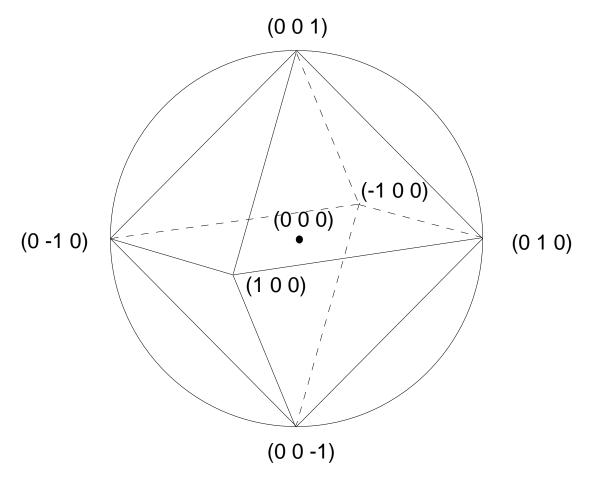


Fig. 1 Pictorial representation of the geometrical domain in which the Wigner and Margenau-Hill quasiprobability distributions take positive values in IR^3 . The octahedron inscribed in the sphere, IR^3 , is the geometrical domain where the quantum characteristic function of the quasiprobability distribution admits a classical trivariate probability mass function. The random variables X_1, X_2, X_3 of the probability mass function produce expectation values which correspond to the expectation values produced by the 3 spin operators S_1, S_2, S_3 , inside the octahedron. The vertices of the octahedron, on the surface of the sphere, represent the pure states of the statistical assembly.

with
$$x_1,x_2,x_3=\pm 1$$
 provided
$$|p_1\pm p_2\pm p_3|\leq 1$$
 and
$$p_1^2+p_2^2+p_3^2\leq 1 \tag{24}$$

We now have the geometrical domain in which the quantum characteristic function of a quasiprobability distribution for the 3 spin operators, admits a probability mass function. Geometrically, $\phi(t_1,t_2,t_3)$ is a characteristic function iff the Bloch vector \overrightarrow{p} lies inside an octahedron inscribed within the sphere given by equation (13), with its center coinciding with the center of the sphere and its vertices touching the sphere at the points $(\pm 1,0,0), (0,\pm 1,0), (0,0,\pm 1)$ as shown in Fig.1. It in understood that the vertices of the octahedron represent pure states. It is to be noted that the classical variates X_1, X_2 and X_3 are generally not independent. They are independent iff any two of the components of the Bloch vector \overrightarrow{p} , p_k 's, are equal to zero. In other words, X_1, X_2 and X_3 are independent iff \overrightarrow{p} lies on one of

the axes. Further, it can be seen that if $p_k = 0$ for some k(k = 1, 2, 3), then X_k is independent of each of the other two random variables.

4 CONCLUDING REMARKS

We have identified the geometrical domain where a classical trivariate probability mass function is admitted by the quantum characteristic function of a quasiprobability distribution of the three spin operators, in IR^3 . The octahedron inscribed in the sphere signifies the domain in which the Wigner and Margenau-Hill quasidistributions assume positive regions and produce expectation values which correspond to the expectation values produced by the normalized, positive classical trivariate probability mass function. It is to be noted that the three random variables of the probability mass function do not imply commutativity. The correspondence between the three noncommuting spin operators and the three random variables of the classical probability mass function is *only* at the expectation value level.

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